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McXtrace 1.4: latest developments in the new release.

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ABSTRACT

This paper presents details on some of the important new features in the newly released version of the x-ray tracing software package McXtrace. Although many developments have been made, this presentation is focused on the features that were required to meet the challenges posed for accurate simulation of the DanMAX beamline — a beamline currently under design at the MAX IV synchrotron. Among these may be mentioned: new source-models, new monochromator crystal models, multilayer capabilities, and the full beamline simulation frame itself.

Keywords: X-ray, simulation, ray tracing, software

1. INTRODUCTION

McXtrace^{1,2} is an open source, x-ray tracing software package designed for simulating any and every x-ray experiment and instrumentation. It was initially released in 2009, but builds on the solid foundation of McStas,³ a very similar tool for neutron ray tracing with a significantly longer history and a proven record. In fact the tools share much of the same code base and workflow. Thus, any user familiar with either can easily switch to the other.

McXtrace operates within the realm of geometrical optics, where ray tracing is directly valid, but since it also tracks the phase of the photons as they travel through the simulation it may be coerced into also handling effects like slit diffraction, etc.¹

A new version, 1.4, of the package has recently been released, which includes numerous improvements over the old version. In summary, the new release includes:

1. A new set of modern, python based GUI and plotting tools
2. Many new components. See section 2 below.
3. An interface to the MCPL-file format.⁴
4. A homogenization of components of similar type, to make it easier for users to switch between models.
5. More standardized installation on debian⁵ class systems.
6. New example simulations.
7. Support for the NeXus-file format

The following is a review of some of the main things that are included in the present release. Firstly, we present a couple of new realistic source models, secondly some optical components, and lastly we show a complete example of beamline simulation: the materials science beamline DanMAX at the MAX IV Synchrotron in Lund, Sweden. The review is focused on the new features that have been built in the process of setting up this complete model of DanMAX.

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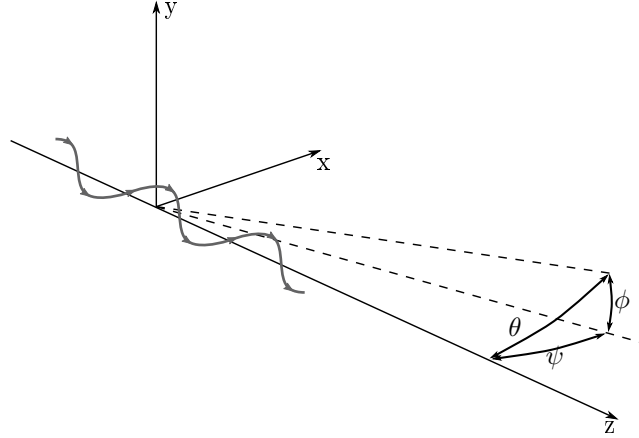


Figure 1. Sketch defining of the parameters θ , ϕ , and ψ from eq. (1)

2. NEW SOURCE COMPONENT MODELS

This section will describe a subset of the new x-ray source component models present in McXtrace version 1.4. In general we find that the new McXtrace models of undulator and bending magnet agrees well with computations performed using other software packages.

2.1 Undulator

The recently included undulator source model is based on the model developed by Kim.⁶ The master equation governing the simulated undulator radiation (in terms of differential flux) is taken to be:

$$\frac{d^2 F_{\sigma,\pi}}{d\Omega d\omega} = \alpha \frac{I}{e} \left(\frac{K\gamma}{1 + K^2/2} \right)^2 \left(\frac{\omega}{\omega_1(0)} \right)^2 N^2 S_N(\omega/\omega_1(\theta)) B_{\sigma,\pi}^2(\omega, \phi, \psi) \quad (1)$$

where K is the dimensionless undulator parameter, α is the fine structure constant, I the storage ring current, e the ring energy, and γ the Lorentz factor. Figure 1 shows the definition of the coordinate system for the radiation and the angle parameters θ , ϕ , and ψ . Furthermore: $\omega_1(\theta) = \frac{2\gamma^2}{1+K^2/2+\gamma^2\theta^2}\omega_u$ is a corrected fundamental angular frequency of the undulator.

The last terms in eq. (1) are defined by eqs. (2) to (4):

$$S_N(\omega/\omega_1(\theta)) = \left(\frac{\sin N\pi\omega/\omega_1(\theta)}{N \sin \pi\omega/\omega_1(\theta)} \right)^2 \quad (2)$$

and

$$\begin{pmatrix} B_{\sigma}(\omega, \phi\psi) \\ B_{\pi}(\omega, \phi\psi) \end{pmatrix} = \frac{1}{\pi} \int_{-\pi}^{\pi} \begin{pmatrix} \psi/K - \cos \xi \\ \phi/K \end{pmatrix} \exp i((\omega/\omega_1(\theta)) \xi - p \sin \xi + q \sin 2\xi) \quad (3)$$

with

$$p(\xi) = 2 \frac{\omega}{\omega_1(0)} \frac{\phi\gamma K}{1 + K^2/2}, \quad q(\xi) = \frac{1}{4} \frac{\omega}{\omega_1(0)} \frac{K^2}{1 + K^2/2} \quad (4)$$

To evaluate the integral in eq. (3), we have used the quadrature routines available from the GNU Scientific Library.⁷ To do so we utilize a new feature of McXtrace, where component developers may easily connect to external libraries through the `DEPENDENCY`-keyword, in the component definition file. In the undulator definition this is written as:

```
DEPENDENCY "-lgsl -lgslcblas"
```

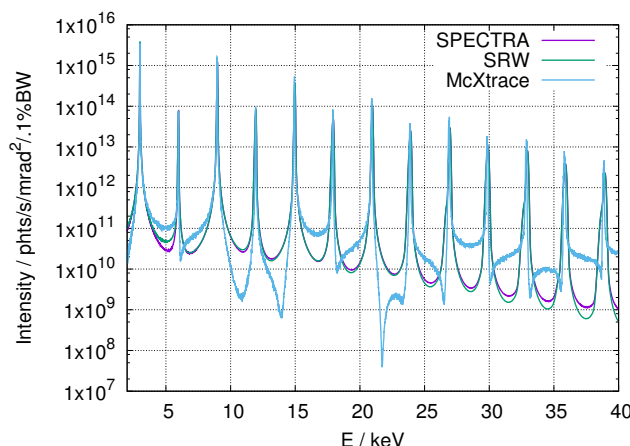


Figure 2. Simulated undulator spectrum for the proposed DanMAX-undulator tuned to a peak at 15 keV. Purple) Sim. with SPECTRA;¹¹ green) Sim. w. SRW;⁹ blue) Sim. w. McXtrace.²

In the creation process the model was tested against proven codes^{8,9,10,11} which are used extensively for undulator radiation. Figure 2 shows a comparison of the radiation spectrum detected 20 m downstream from an undulator with the same parameters as the one currently under order for the DanMAX¹² (IVU16) (See section 4) beamline at MAX IV Laboratory.¹³ This undulator is ≈ 3 m long, with a period of 16 mm, corresponding to 187 undulator periods. For this test, the undulator was tuned to emit radiation at 15 keV. Given the ring parameters of the 3 GeV storage ring at MAX IV, this sets the undulator gap to ≈ 6.01 mm, which in turn yields a peak magnetic field at the undulator centre of 0.8363 T (or in terms of undulator parameter $K = 1.249$). On-peak characteristics match quite well across computer codes, whereas the description at half periods differs significantly. In many cases this accuracy is quite sufficient owing to the high ratio between peak and valley flux.

To include emittance effects originating from an imperfect electron beam in the storage ring we employ a simple Monte Carlo scheme in line with the general philosophy and design of McXtrace (and other x-ray tracing tools), and simply add normally distributed errors to both the origin of the ray and its direction. In terms of fig. 1, this amounts to adding normally distributed errors to the origin and the angles ϕ and ψ . We have validated the procedure against computations with identical parameters in SPECTRA and found the result to agree satisfactorily (See figs. 3 and 4).

2.2 Bending Magnet

Further to the completeness of the set of available source models in McXtrace, we distribute a bending magnet source. Based on a simplified approach¹⁴ it is very efficient and provides a fairly accurate description of radiation from a bending magnet source within the central cone of radiation. A comparison between the McXtrace description and simulations using SPECTRA is shown in fig. 5. Clearly, the two descriptions agree to a very high degree.

3. NEW OPTICS COMPONENTS

In this section we present some of the the main new/improved optics components in McXtrace.

3.1 Mirrors

The distribution now includes models of mirrors including an easy to use flat perfectly flat mirror, as well as a toroidally bent mirror. The toroid may be focusing or defocusing depending on the signs of the bending radii. This is useful e.g. when the effect of heat-load induced bumps is investigated. All mirrors can now take as input an external reflectivity file, which may be resolved in energy and incidence angle or simply q . This gives the simulator the option of computing reflectivities using specialized software, e.g. IMD which has found widespread use in the astrophysics community. Through this we can easily include multilayer coatings in the simulations.

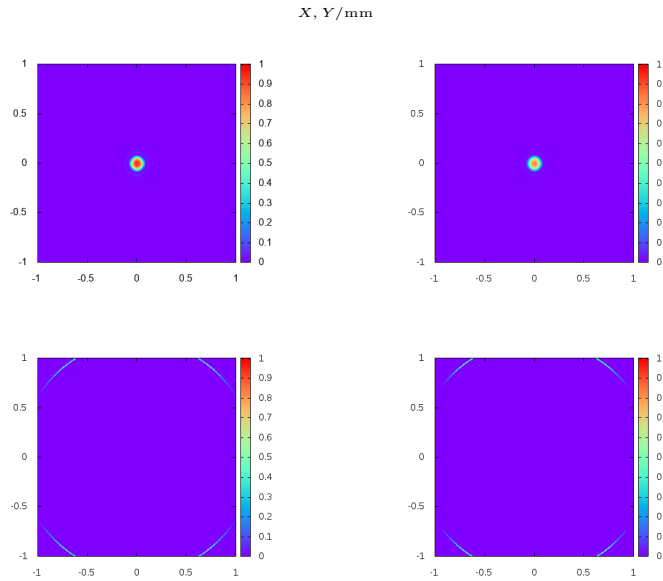


Figure 3. Comparison of the spatial distribution of undulator radiation 20 m downstream from an undulator of the IVU16 type in the MAX-IV storage ring, where the undulator has been tuned to have its 11th harmonic peak at 33 keV. The left column is calculations done in SPECTRA, the right is done with the undulator model in McXtrace. Top row is on-peak radiation (33 keV), bottom row is an example of off-peak radiation at 25.3 keV. The peak intensity has been normalized to 1.

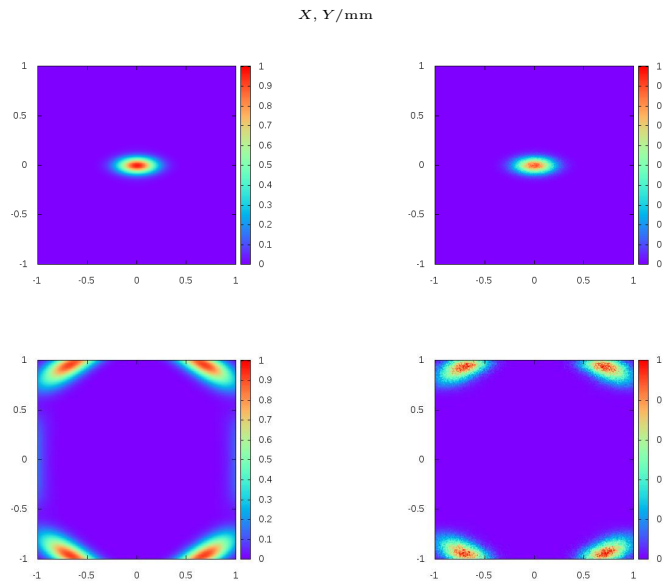


Figure 4. Comparison of the spatial distribution of undulator radiation, *with* the inclusion of emittance from an imperfect electron beam, measured 20 m downstream from an undulator of the IVU16 type in the MAX-IV storage ring, where the undulator has been tuned to have its 11th harmonic peak at 33 keV. The left column is calculations done in SPECTRA, the right is done with the undulator model in McXtrace. Top row is on-peak radiation (33 keV), bottom row is an example of off-peak radiation at 25.3 keV. The peak intensity has been normalized to 1.

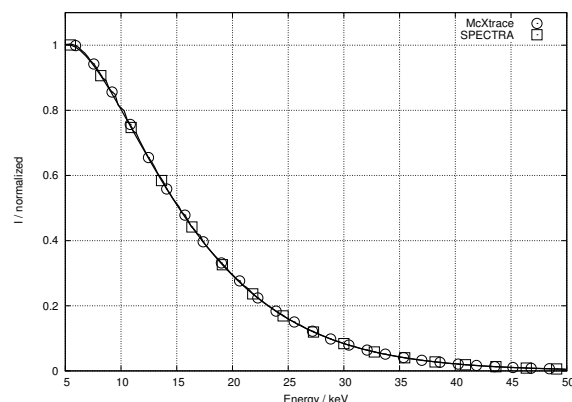


Figure 5. Comparison between energy spectra of SPECTRA (squares) and McXtrace (circles) bending magnet models. The bending magnet is assumed to have a 0.6 T and to be in a 2.4 GeV, 0.4 mA storage ring. Energy spread and emittance effects have been neglected.

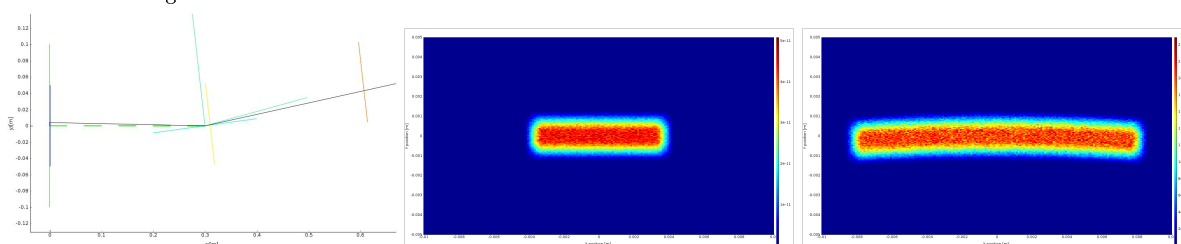


Figure 6. Left) Sketch of a raytracing example with mirror directly from the `mxdisplay`-tool shipped with McXtrace. The area plots (middle and right) show the intensity distribution of a flat uniform source reflected in a mirror and monitored 1 m downstream. The edges are not sharp in either plot due to divergence in the source model. Middle) Flat mirror. Right) Toroidal mirror with radii 20 m and 0.01 m.

The model of the DanMAX-beamline (See section 4.) includes a double bounce multilayer monochromator, where the first element is modelled by interchangeable bent and flat mirrors. The former is used where the full white beam impinges on the first multilayer resulting in a heat-bump; the latter when the beam has been pre-monochromatized and no heat-bump is generated. A bottleneck when simulating mirrors with coatings, has been file IO, in particular for multilayers where high energy and angle resolution is often required. This is now less cumbersome due to a scheme where a datafile may be shared among otherwise independent beamline components.

3.2 Monochromator Crystals

Simulating monochromator crystals in McXtrace may be done using the two new components `Bragg_crystal.comp` and `Bragg_crystal_bent.comp`. The models are currently limited to single-atom crystals with cubic space-groups. We have compared the characteristics of crystals models against XOP¹⁵ and analytical calculations,¹⁶ which generally shows very good agreement as shown in fig. 7. A small offset to the peak location, on the order of 0.1 eV, remains between the perfectly flat crystal models. This may be attributed to different crystallographic standards in XOP and McXtrace, when describing the atomic distances of crystalline Si.

4. SIMULATION EXAMPLE: DANMAX

As a tool in the design process of the DanMAX beamline at the MAX IV synchrotron, we have developed a complete McXtrace-model of the beamline. The model has helped make decisions on various issues, and is tracking design changes as they happen (for instance due to engineering realities). Figure 8 shows a sketch of the beamline layout, where the central components have been included. The beamline will serve as both an imaging as well as a powder diffraction beamline. A unique feature of this beamline is the use of a double bounce multilayer monochromator (DMM) in conjunction with a standard high-resolution double crystal monochromator

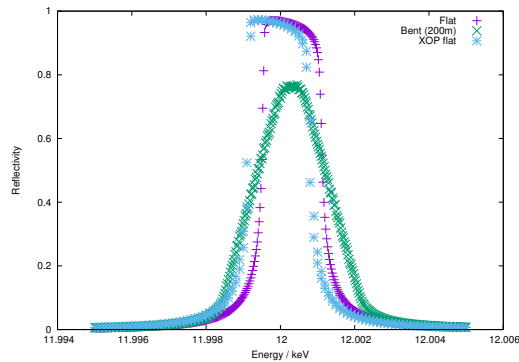


Figure 7. Spectra of radiation reflected by a Si 111-monochromator tuned to 12 keV. The radiation illuminating the crystals is uniformly distributed in energy and fully collimated. Purple corresponds to a perfectly flat crystal, green to a crystal bent to a radius of 200m, and blue to a flat crystal simulated by XOP. The slight difference in central energy is due to mismatching crystallographic descriptions of Si.

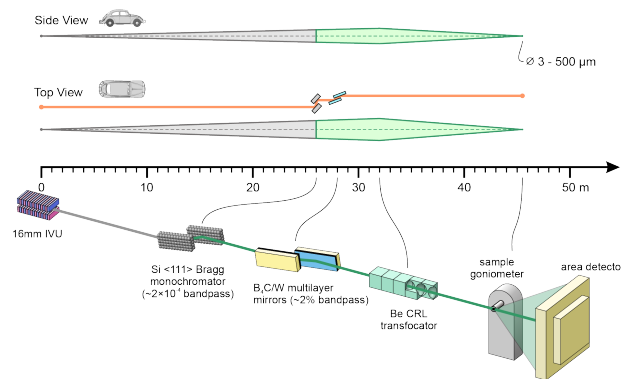


Figure 8. Cartoon of the DanMAX beamline optical concept.

(DCM). When the DCM is active the DMM may be used for higher harmonic suppression. To exemplify: if the DCM is tuned to 15 keV simulations indicate that the harmonic at 45 keV is suppressed by 11 orders of magnitude (fig. 9). Figure 10 shows examples of data that may be expected at DanMAX where the real beamline parameters for e.g. source, detector pixels, heat load corrections etc. have been included.

5. INFRASTRUCTURE IMPROVEMENTS

5.1 New GUI

A new Python/Qt based GUI is available for McXtrace. Section 5.1 shows examples of the new simulation GUI (left) and of the new plotting tool. Also included in the new GUI is an improved editor based on QScintilla. A novel feature is the predictive text editors helping users write instrument files.

6. ACKNOWLEDGEMENTS

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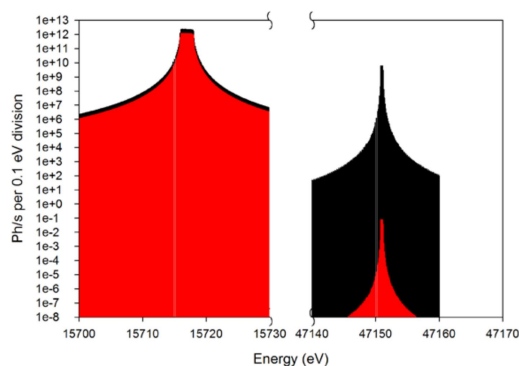


Figure 9. Higher harmonic suppression using a double bounce multilayer monochromator. Double crystal monochromator is tuned to a Bragg angle corresponding to 15 keV. The black curve shows the simulated photon flux without the double bounce multilayer monochromator, the red curves show the flux *with* the multilayer in. We find a higher harmonic rejection ratio of $\approx 10^{14}$.

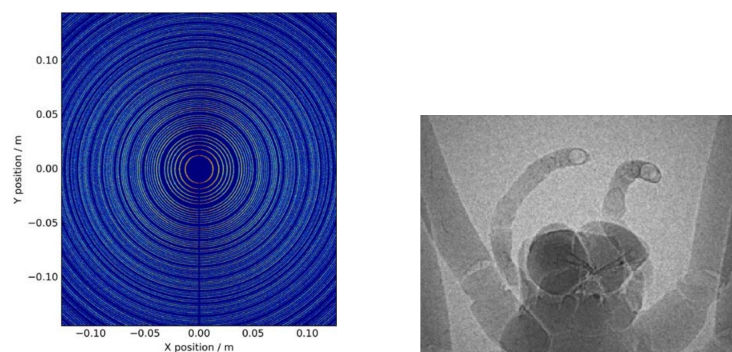


Figure 10. Examples of results obtained with the virtual DanMAX-beamline as simulated with McXtrace. Left) Standard powder diffraction pattern from an LaB₆-powder. Right) Absorption contrast image of the head of a spider.

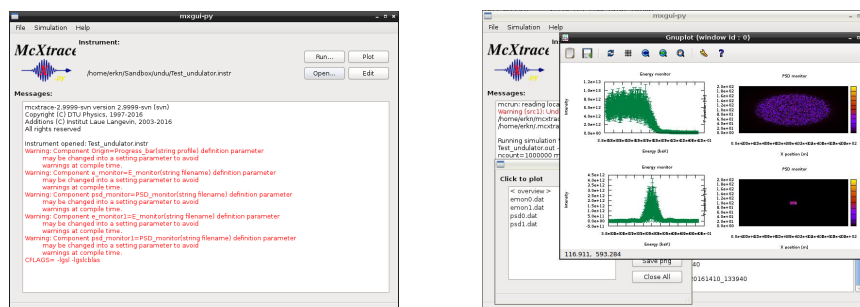


Figure 11. Examples of the new McXtrace python/Qt based GUI. Left) The main window. Right) plotting windows.

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